# Artificial Neural Networks to Extract Optical Properties of Marine Microorganisms from their Mueller Scattering Matrix

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## LONG-TERM GOAL

The long term goals of this project are to understand and quantify light scattering from ensembles of both spherical and non-spherical objects in ocean water, to characterize the effect of ensembles of micro-organisms and inorganic particulates on the propagation of polarized light through sea water, and to assess the feasibility of computer simulated artificial neural networks to extract optical properties of marine particulates from polarized light scattering measurements.

## OBJECTIVES

The scientific objectives of this project are to develop numerical or analytical models that predict angle-dependent scattering of polarized light from ensembles of non-spherical marine organisms, detritus, and inorganic particulates, and to verify and examine the validity and range of applications of the models by comparison with exact calculations and/or experimental results. Specific tasks toward these objectives are:

(1) to develop an artificial neural network to recognize features in the Mueller matrix elements associated with the optical properties, size distribution, and irregular shape of ocean scatterers,

(2) to make experimental measurements in the laboratory of light scattering from samples of micro-organisms and inorganic particles in ocean water, and

(3) to continue to refine and enhance analytical models such as the coupled-dipole method for predicting polarized light scattering from non-spherical particles.

## APPROACH

The bulk of our past efforts have been in training neural networks to extract optical properties, particularly size parameter, from collections of microscopic particles in sea water (Hull and Quinby-Hunt, 1996,1998.) During the current reporting period we have shifted focus to aerosols because of an opportunity to test a neural network in an instrument. Hunt, *et al.* (1998,1999) have built and are now testing a light scattering instrument (the DPS) at Berkeley Lab for determining the size distribution and complex index of refraction of microscopic particles suspended in air. In this instrument, the aerosol is passed through a scanning polarization-modulated nephelometer that measures directly three Mueller matrix elements as functions of scattering angle. The size distribution and complex index of refraction are then calculated by simultaneously fitting these three functions with Mie scattering calculations. An accurate

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analysis of the scattering data from the DPS requires that the microscopic particles be well-modeled by spheres. A neural network trained using Mie calculations for a range of size distributions and complex indices of refraction is an alternative to curve fitting, but still requires that the particles be very nearly spherical. The advantage of using neural networks, however, is that they do not require detailed, explicit functions or curve fitting, but rather they learn by example. Experimental data or calculations based on approximation methods such as the coupled-dipole model can provide input data for a range of particle shapes as well as optical properties. Coupled-dipole calculations are much too computer-intensive to use them in a curve-fitting routine, however, a data base could be created and used to train a neural network to avoid carrying out extensive calculations for each measurement. It is important to first determine the accuracy of a neural network to make predictions for a simple and well-defined system of spherical particles before applying it a more complex problem.

Creating and evaluating a neural network requires several steps. The first step was to prepare a data base. We used Mie calculations of the scattering matrix elements in order to provide well-characterized training data for the neural networks. All calculations were made for a log-normal distribution of sphere sizes, a physically realistic distribution for microscopic particles (Quinby-Hunt, *et al.*, 1999.) The equation below is the distribution function used in the calculations. In this equation, $x$ is the particle diameter and $N(x)$ is the number density of particles having a given diameter, $x$. The quantity $x_m$ is the average value of the particle diameter and $\sigma_g$ is the standard deviation of log$x$.

$$N(x) = \frac{1}{x\sigma_g^2\sqrt{2\pi}} \exp\left[\frac{-(\log x - \log x_m)^2}{2\sigma_g^2}\right]$$

Graphs of this function for several values of peak particle diameter and standard deviation are shown in Figure 1 below.

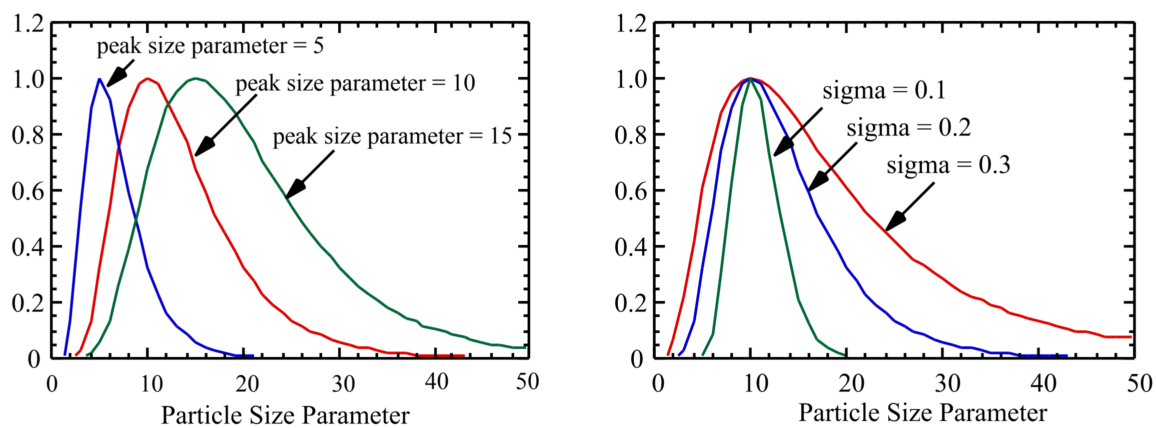


Figure 1. Log normal distribution functions similar to those used in the Mie calculations. Size parameter is shown rather than particle diameter. Graph on the left shows peak values in size parameter of 5, 10 and 15 each with the same deviation, sigma of 0.20. The graph on the right shows three different values of sigma, 0.10, 0.20 and 0.30, each with a peak size parameter of 10.

## WORK COMPLETED

Training and testing sets for the networks were constructed from Mie calculations by varying the mean diameter (defined for the log-normal distribution) from 0.09 to 0.20 in steps of 0.10, the geometric mean standard deviation from 0.10 to 0.50 in steps of 0.10, the relative index of refraction from 1.33 to 1.52 in steps of 0.03, and the absorption coefficient from 0.05 to 0.20 in steps of 0.05. These ranges for the four parameters were selected because they included all experimental values that have been measured with the DPS. Approximately 400 data sets were calculated from randomly selected combinations of the four parameters. We constructed a 16-element column vector for each Mie calculation. Since we wish to eventually use the network to analyze light scattering data from the DPS, we chose elements corresponding to those measured in the instrument. The measurement were the total intensity, $S_{11}$, and the normalized matrix elements $S_{12}$ and $S_{34}$ (in 10° increments from 30° to 150°.) We chose the first element in the training vector to be the difference between the logs of two values of the total intensity, $\mathrm{Log}S_{11}(30°)$-$\mathrm{Log}S_{11}(150°)$, elements 2 through 6 to be $S_{12}$ for angles 70° through 110°, and the remaining 10 elements to be $S_{34}$ at angles 50° through 150°. A training or testing set consisted of a matrix made up of many of these column vectors.

The data was prepared by performing a principal component analysis to remove redundancies in the data or duplicate (or near duplicate) input vectors. We retained those principal components in the vectors which accounted for 99.9% of the variation in the data set. The resulting input vectors were considerably reduced in number of elements, but no duplicate vectors were found. Training with the transformed data set resulted in a small reduction in the accuracy of the network, but it was important to keep the number of input data points as small as possible so that the network training could be carried out on a desktop computer. Experience has shown that at least 3 or 4 processing elements for each input data point is required for a network to have sufficient power to solve a problem of the type of interest here (Beale and Jackson, 1990, McCord and Illiangworth, 1991, Hagan and Beale, 1996.) Half of the resulting vectors were used to train the network, one-fourth were used to validate the training as it progressed and one-fourth were used to test the final network.

The next step was to create a network and train it. The network design we selected was a two-hidden layer back propagation network. The number of neurons in the first hidden layer was varied from 25 to 80 and the number of neurons in the second hidden layer was varied from 6 to 16. Levenburg-Marquardt optimization, a gradient descent method, was used to train the networks. Computations such as selection of initial weight matrices, summing weighted inputs (matrix inner product), calculations of the transfer functions, applying learning rules, and assessing the network's learning rate and performance were carried out using algorithms in the MATLAB library and its associated Neural Network Toolbox (Demuth and Beale, 1998.)

Finally, we performed an analysis of the network performance. We put all the vectors (training, validation, and test sets) through the network and performed a linear regression between the outputs and the corresponding targets for each of the four parameters, mean particle diameter, standard deviation, index of refraction, and absorption. A number of network training methods such as increasing the number training cycles or the number of neurons in each hidden layer were used to improve the performance of the network.

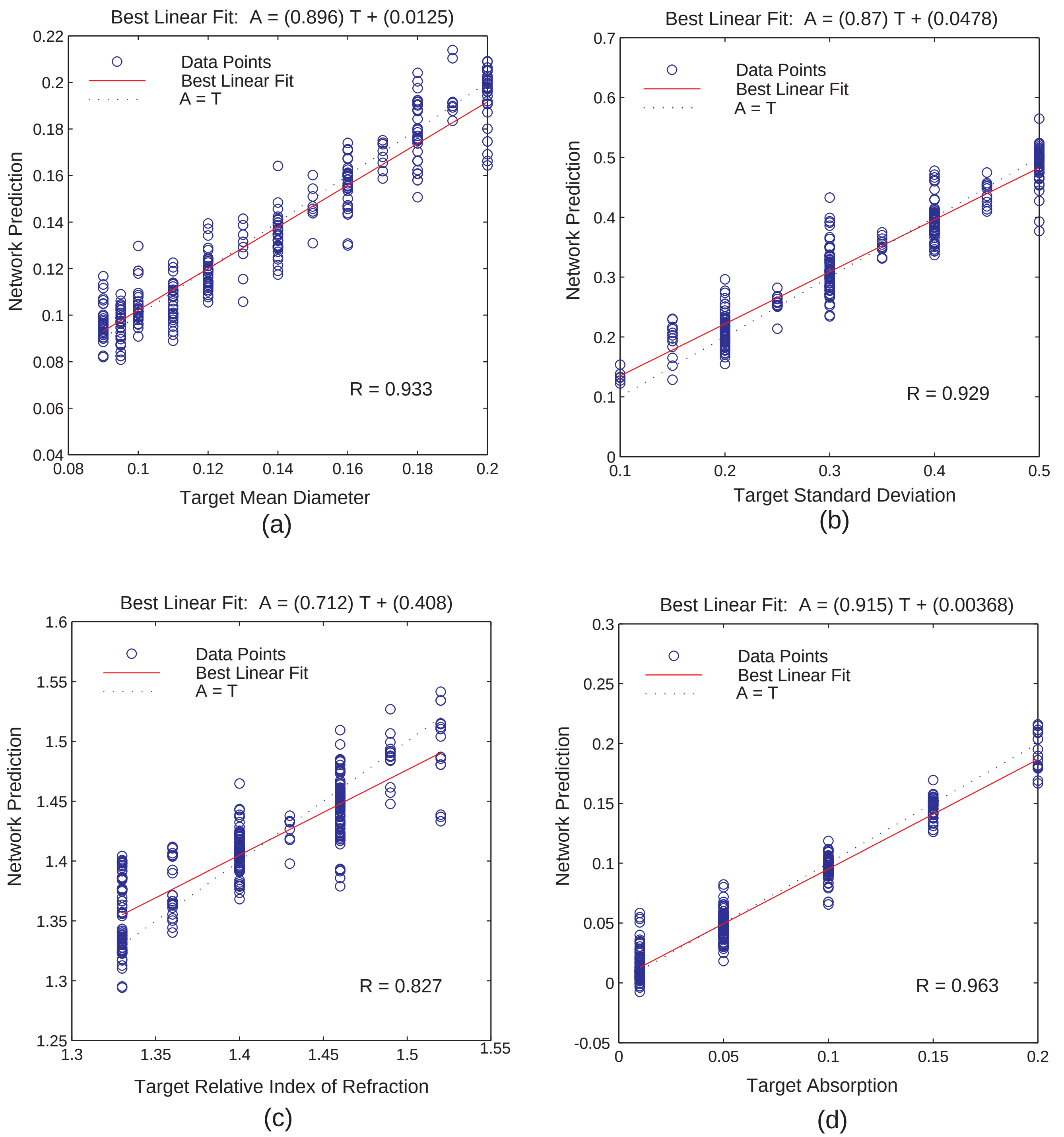


Figure 2. Analysis of network response. Entire data set (training, validation, and testing) was put through a trained network of 60 neurons in first layer and 12 neuron in second layer. A linear regression between network outputs and the corresponding targets was performed. Figure 2(a) shows the results for the mean diameter of the particle collection, (b) shows the results for the standard deviation in the log of diameter, (c) shows the results for relative index of refraction, and (d) shows the results for absorption.

## RESULTS

The component analysis of our input vectors indicated a considerable redundancy in the elements and reduced the number of elements from 16 to only 6. An analysis of input data for a wider range of particle sizes would probably have a very different outcome. A faster computer with memory upgrades, together with improved and more efficient algorithms for training and evaluating neural networks allowed us to construct a single network that predicted three parameters, mean diameter, standard deviation, and absorption parameters with a confidence (R-value) of greater than 0.9. The fourth parameter, index of refraction, proved to be a more difficult problem. The greatest R-value we were able to obtain was about 0.84. Increasing the number of neuron past 60 in the first layer did not improve the network performance. In fact, the performance tended to worsen. Figure 2 shows the results of a linear regression between network outputs and the targets for 320 input vectors for a network of 60 neurons in the first hidden layer, and 12 neurons in the second hidden layer. There is still a lot scatter in the network predictions. The strong effects of variations in size parameter tend to mask the more subtle changes the matrix elements due to variations in index of refraction, sigma, and absorption. Generally, networks for predicting these parameters were successful only for small ranges of size parameter.

## IMPACT/APPLICATION

While it is not certain from the work presented here, that neural networks can replace curve-fitting techniques in instruments measuring the light scattering from aerosols, they are reliable enough at this point to be used to filter the data. They certainly provide good starting values for the parameters that can reduce the number of computations necessary to fit scattering data. Furthermore, other network designs and training techniques not yet tried with light scattering data may well improve the performance to a reliable level. It is also important to note that the performance of the neural network is much better for microscopic particles in sea water due to the much smaller value of the index of refraction than for particles in air. A light scattering instrument that can determine the average diameter, the standard deviation, the relative index of refraction, and the absorption for a suspension of microscopic particles from light scattering measurements analyzed by a neural network is possible.

## TRANSITIONS

The following projects make use of computer software and/or experimental methods developed in this research for measuring and modeling the light scattering by irregularly shaped particles:

1 - A version of the coupled-dipole approximation is being used in a project funded by DOE at Berkeley Lab for modeling soot particles in diesel exhaust. The goal of that project is to develop an instrument, possibly using a neural network, for measuring sizes and optical properties of the soot particles.

2 - In another DOE funded project at Berkeley Lab, experimental methods developed by this project are being used to help design an instrument for on-line measurement of the alignment of the fibers in paper production.

## RELATED PROJECTS

This work was a component of past ONR-sponsored projects and is related to a current project by Hunt and Quinby-Hunt at Berkeley Lab for the measurement of light scattering in both seawater and the sea-air boundary layer, and calculations of light scattering from non-spherical aerosol particles using parallel processing.

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